1 Review of useful concepts and Introduction

1.1 Multivariate Gaussian

$f(x) = \frac{1}{2\pi\sqrt{|\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$

Suppose we have a Gaussian random vector $X_V \sim N(\mu_V, \Sigma_{VV})$.

Suppose we take two disjoint subsets of V: $A = i_1, ..., i_k$ and $B = j_1, ..., j_m$.

Then, the conditional distribution:

$P(X_A|X_B = x_B) = N(\mu_{A|B}, \Sigma_{A|B})$ is Gaussian:

$\mu_{A|B} = \mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(x_B - \mu_B)$

$\Sigma_{A|B} = \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}$

1.2 Convex / Jensen's inequality

g(x) is convex $\Leftrightarrow x_1, x_2 \in \mathbb{R}, \lambda \in [0,1] : g''(x) > 0$

$g(\lambda x_1 + (1-\lambda)x_2) \leq \lambda g(x_1) + (1-\lambda)g(x_2)$

$\varphi(\mathrm{E}[X]) \leq \mathrm{E}[\varphi(X)]$

1.3 Review Probability

Probability space (Ω, F, P)**:** Set of atomic events Ω. Set of all non-atomic events (σ-Algebra): $F \in 2^{\Omega}$. Probability measure: $P : F \rightarrow [0,1]$

Bayes' rule: $P(B|A) = P(A,B)/P(A) = P(A|B)P(B)/P(A)$, where $P(A) = \sum_b P(A|B)P(A)$

Union: $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

Rules for joint distributions:

Sum rule (Marginalization):

$P(X_{1:i-1}, X_{i+1:n}) = \sum_{x_i} P(X_{1:i-1}, X_i = x_i, X_{i+1:n})$

Product rule (Chain rule):

$P(X_{1:n}) = P(x_1)P(X_2|X_1)...P(X_n|X_{1:n-1})$

Conditional Independence:

$X \perp Y|Z$ iff $P(X,Y|Z) = P(X|Z)P(Y|Z)$

If $P(Y|Z) > 0 \Rightarrow P(X|Z,Y) = P(X|Z)$

Properties of Conditional Independence:

Symmetry: $X \perp Y \mid Z \Rightarrow Y \perp X \mid Z$

Decomposition: $X \perp (Y,W) \mid Z \Rightarrow X \perp Y \mid Z$

Contraction: $(X \perp Y \mid Z) \wedge (X \perp W \mid Y,Z) \Rightarrow X \perp Y,W \mid Z$

Weak union: $X \perp Y,W \mid Z \Rightarrow X \perp Y \mid Z,W$

Intersection: $(X \perp Y \mid W,Z) \wedge (X \perp W \mid Y,Z) \Rightarrow X \perp Y,W \mid Z$

2 Bayesian Networks

2.1 Basic concepts

A Bayesian network (G,P) consists of:

- A BN structure G (directed, acyclic graph)
- A set of conditional probability distributions
- (G,P) defines the joint distribution: $P(X_1,...,X_n) = \prod_i P(X_i|Pa_{X_i})$

BNs with 3 nodes:

2.2 Active trails and d-separation

An undirected path in a BN structure G is called active trail for observed variables $O \in X_1, ..., X_n$ of for every consecutive triple of variables X, Y, Z on the path:

- **indirect causal effect**: $X \rightarrow Y \rightarrow Z$ and Y unobserved
- **indirect evidential effect**: $X \leftarrow Y \leftarrow Z$ and Y unobserved
- **common cause**: $X \leftarrow Y \rightarrow Z$ and Y unobserved.
- **common effect**: $X \rightarrow Y \leftarrow Z$ and Y or any of Y's descendants is observed.

Any variables X_i and X_j for which there is no active trail for observations O are called d-separated by O.

Theorem: $d - sep(X_i; X_j|O)) \quad \Rightarrow X \perp Y|Z$

Converse does not hold in general!

3 Exact inference (tree-structured BN)

3.1 Variable elimination

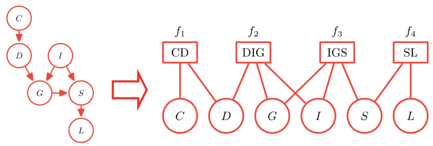
- Given a BN and query $P(X|E = e)$
- Choose an ordering of $X_1, ..., X_n$ **Eliminate variables from the outside in!**
- Set up initial factors: $f_i = P(X_i|Pa_i)$
- For $i = 1 : n, X_i \notin X, E$
  - Collect and multiply all factors f that include X_i
  - Generate new factor by marginalizing out X_i: $g_{X\,i} = \sum_{x_i} \prod_j f_j$
  - Add g to set of factors
- Renormalize $P(x,e)$ to get $P(x|e)$

Variable elimination for polytrees:

- Pick a root, (avoiding X and E)
- Orient edges towards root
- Eliminate variables according to topological order

3.2 Avoiding recomputation: factor graphs

FG for a BN is a bipartite graph consisting of variables (circles) and factors (rectangles). **It is not a unique representation.**



3.2.1 Sum-product/Belief Propagation (BP) Algorithm:

- Initialize all messages as uniform distribution
- Until converged to:
  - Pick a root in the factor graph and reorient the edges towards this root.
  - Update messages according to this ordering. Do passes from leaves to root and from root to leaves.
- If a leaf node is a variable node: $\mu_{x \rightarrow f}(x) = 1$ -

If a leaf node is a factor node: $\mu_{f \rightarrow x}(x) = f(x)$ -

Messages from node v to factor u:

$\mu_{v \rightarrow u}(x_v) = \prod_{u' \in N(v)\setminus\{u\}} \mu_{u' \rightarrow v(x_v)}$

- Messages from factor u to node v:

$\mu_{u \rightarrow v}(x_v) = \sum_{x_u \sim x_v} f_u(x_u) \prod_{v' \in N(u)\setminus\{v\}} \mu_{v' \rightarrow u(x'_v)}$

  - Break once all messages change by $\leq \epsilon$

Hope: after convergence, we have:

$P(X_v = x_v) = \frac{1}{Z}\prod_{u \in N(v)} \mu_{u \rightarrow v}(x_v)$

$P(\overrightarrow{X_u} = \overrightarrow{x_u}) = \frac{1}{Z} f_u(\overrightarrow{x_u}) \prod_{v \in N(u)} \mu_{v \rightarrow u}(x_v)$

If we have a polytree Bayesian network:

- Choose one node as root
- Send messages from leaves to root and from root to leaves

4 Approximate inference (loopy networks)

With loopy graphs, BP is often **overconfident/oscillates**.

4.1 Variable elimination for MPE (most probable explanation):

- Given BN and evidence E=e
- Choose an ordering of $X_1, ... x_n$
- Set up initial factors $f_i = P(X_i|Pa_i)$
- For $i = 1 : n, X_i \notin E$:
  - Collect and multiply all factors f_j that include X_i
  - Generate new factor by maximizing out X_i: $g_i = \max_{w=x_i} \prod_j f_j$
  - Add g to set of factors
- For $i = n-1 : 1, X_i \notin E$: $\hat{x}_i = \underset{x_i}{\mathrm{argmax}}\, g_i(x_i, \hat{x}_{i+1:n})$

Retrieving MAP from Max-Product (MAP = MPE for a subset of RVs):

- Define max-marginals:

$P_{max}(X_v = x_v) := \max_{x \sim x_v} P(x)$

- For tree factor graphs, max-product computes max-marginals:

$P_{max}(X_v = x_v) \propto \prod_{u \in N(v)} \mu_{u \rightarrow v}(x_v)$

- Can retrieve MAP solution from these (must be careful when ties need to be broken).

4.2 Sampling based inference: compute marginals as expectations

Hoeffding's inequality: Suppose f is bounded in $[0, C]$. Then:

$P(|E_P[f(X)] - \frac{1}{N}\sum_{i=1}^N f(x_i)| \geq \epsilon) \leq 2exp\left(\frac{-2N\epsilon^2}{C^2}\right)$

Monte Carlo Sampling from a BN:

- Sort variables in topological ordering X_1, X_n
- For $i = 1$ to n, sample: $x_i \sim P(X_1 = x_1, ..., X_{i-1} = x_{i-1})$

Rejection Sampling:

- Collect samples over all variables:

$\hat{P}(X_A = x + A|X_B = x_B) = \frac{Count(x_A, x_B)}{Count(x_B)}$

- Throw away samples that disagree with x_B
- Count fraction of x_a on remaining samples

4.2.1 Directly sampling from the posterior: MCMC

Markov Chain:: A (stationary) MC is a sequence of RVs $X_1, ..., X_N$, with prior $P(X_1)$ and transition probabilities $P(X_{t+1}|X_t)$ independent of t.

Markov assumpt.: $X_{1:t-1} \perp X_{t+1:T}|X_t, \forall t > 1$

Stationarity assumption:

$P(X_{t+1} = x|X_t = x') = P(X_t = x|X_{t-1} = x'), \forall t > 1$

If ergodic (= there exists a finite t such that every state can be reached in exactly t steps), then: it has a unique and positive stationary distribution $\pi(X) > 0$, such for all x: $\lim_{N \rightarrow \infty} P(X_N = x) = \pi(x)$ and $\pi(X) \perp P(X_1)$.

If MC satisfies the **detailed balance equation** (for unnormalized distribution Q, for all x, x': $Q(x)P(x'|x) = Q(x')P(x|x')$), then the MC has stationarity distribution $\pi(X) = 1/Z\,Q(X)$.

Designing Markov Chains:

- Proposal distribution $R(X'|X)$: given $X_t = x$, sample "proposal"$x' \sim R(X'|X = x)$
- Acceptance distribution
  - Suppose $X_t = x$
  - With probability $\alpha = min\left\{1, \frac{Q(x')R(x|x')}{Q(x)R(x'|x)}\right\}$ set: $X_{t+1} = x'$
  - With probability $1 - \alpha$, set $X_{t+1} = x$

MCMC for graphical models: Gibbs sampling (Random Vs Practical variant):

- Start with initial assignment x to all variables
- Fix observed variables $X_B = x_B$
- For $t = 1$ to ∞, do:
  - Pick a variable i uniformly at random from $\{1, ..., n\} \setminus B$ / Set ordering, and then, for each X_i (except those in B)
  - Set v_i = values of all x except x_i
  - Sample x_i from $P(X_i|v_i)$

5 Dynamical models (include time)

5.1 Examples with one variable per time step

$X_1, ..., X_T$ (unobserved) hidden states

$Y_1, ..., Y_T$ (noisy) observations

HMMs (polytrees: can use belief propagation): X_i categorical, Y_i categorical (or arbitrary)

Kalman filters: X_i, Y_i Gaussian distributions

- $P(X_1)$: prior belief about location at time i
- $P(X_{t+1}|X_t)$: **'Motion model'** (how do I expect my target to move in the environment?): $X_{t+1} = FX + \epsilon_t$ where $\epsilon_t \sim N(0, \Sigma_x)$
- $P(Y_t|X_t)$: **'Sensor model'** (what do I observe if target is at location X_t?) $Y_t = HX_t + \eta_t$ where $\eta_t \sim N(0, \Sigma_y)$

5.2 Inference tasks

Filtering: $P(X_t|y_{1,...,t})$ Is it raining today?

Prediction: $P(X_{t+\tau}|Y_{1:t})$ Rain 5 days from now?

Example for one step: $P(X_{t+1}|Y_{1:t}) = \sum_x P(X_{t+1}, X_t = x_t|Y_{1:t}) = \sum_x P(X_{t+1}|X_t = x_t)P(X_t|Y_{1:t})$ (with KFs, you need **integrals**!)

Smoothing: $P(X_\tau|y_{1:t})$ with $\tau < t$ Did it rain

last week? [Can use sum-product (aka forward-backward).]
MPE: $\underset{x_{1:T}}{argmax} P(x_{1:T}|y_{1:T})$ Can use max product (aka Viterbi algorithm).
Bayesian filtering: Start with $P(X_1)$:
At time t, assume we have $P(X_t|y_{1:t-1})$
Conditioning: $P(X_t|y_{1:t}) = \frac{P(X_t|y_{1:t-1})P(y_t|X_t)}{\sum_{x_t} P(X_t|y_{1:t-1})P(y_t|X_t)}$
Prediction ($O(n^2)$ vs $O(n)$ in conditioning):
$P(X_{t+1}|y_{1:t}) = \sum_x P(X_{t+1}|X_t)P(X_t|y_{1:t})$
Since HMM is a polytree, smoothing/MPE can be computed by VE/BP. Kalman filtering: Bayesian filtering for continuous problems. RV corrupted by Gaussian distributions with zero mean. **Bayesian filtering is basically the same, except that sums turn to integrals. General Kalman update**
- Transition model: $P(x_{t+1}|x_t) = N(x_{t+1}; Fx_t, \Sigma_x)$
- Sensor model: $P(y_t|x_t) = N(y_t; Hx_t, \Sigma_y)$
- Kalman update:
$\mu_{t+1} = F\mu_t + K_{t+1}(y_{t+1} - HF\mu_t)$
$\Sigma_{t+1} = (I - K_{t+1})(F\Sigma_t F^T + \Sigma_x)$
- Kalman gain: $K_{t+1} = (F\Sigma_t F^T + \Sigma_x)H^T(H(F\Sigma_t F^T + \Sigma_x)H^T + \Sigma_y)^{-1}$

5.3 Examples with > 1 variable per time step

Dynamic Bayesian Networks: a BN at every time step
These models typically have many loops. Exact inference is usually intractable.

5.4 Approx. infer. for filtering (DBNs and non-linear Kalman filters): Particle filtering

Suppose: $P(X_t|y_{1:t}) \approx \frac{1}{N}\sum_{i=1}^N \delta_{x_{i,t}}$, where δ is the indicator function. **Prediction**: Propagate each particle: $x_i' \sim P(X_{t+1}|x_{i,t})$
Conditioning:
- weight particles $w_i = \frac{1}{Z}P(y_{t+1}|x_i')$
- resample N particles $x_{i,t+1} \sim \frac{1}{Z}\sum_{i=1}^N w_i \delta_{x_i'}$

Conclusion we came to: $Z = \sum_{i=1}^N w_i \delta_{x_i}$

6 Probabilistic Planning

6.1 Markov Decision Processes

An MDP is specified by a quintuple: $(X, A, r, P(x'|x,a), \gamma)$, where X are states, A are actions, $r(x,a)$ is a reward function and transition probabilities:
$P(x'|x,a) = \text{Prob(Next state} = x'|\text{Action } a)$
Objective: find a stationary policy $\pi : S \to A$ that maximizes the sum of cumulative rewards.
Value of a state given a policy : sum of cumulative rewards, given that the initial state is this state $\to$ **Bellman equation:**
$V^\pi(s) = \mathbb{E}\Big[\sum_{t=0}^\infty \gamma^t r(s_t, \pi(s_t), s_{t+1})|s_0 = s\Big]$
$= \sum_{s'\in S} P(s'|s,\pi(s))\Big[r(s,\pi(s),s') + \gamma V^\pi(s')\Big]$
$= r(s,\pi(s)) + \gamma\sum_{s'\in S} P(s'|s,\pi(s))V^\pi(s')$
Theorem (Bellman): a policy is optimal iff it is greedy w.r.t. its induced value function!
$V^*(x) = max_a[r(x,a) + \gamma\sum_{x'} P(x'|x,a)V^*(x')]$
Bellman equation mais geral:
$V^*(x) = max_a[\sum_{x'} P(x'|x,a)(r(a,x,x') + \gamma V^*(x')])$
Optimal policy:
$\pi^*(s) = \underset{a\in A}{argmax}[r(x,a) + \gamma\sum_{x'} P(x'|x,a)V^*(x')]$

6.2 Policy iteration (Cost $O(S^3 + SA\Delta)$)

Start with an arbitrary (e.g. random) policy π. Until converged, do:
- Compute value function $V^\pi(x)$
- Compute greedy policy π_G w.r.t. V^π
- Set $\pi \leftarrow \pi_G$

Guaranteed to monotonically improve and to converge to an **optimal** policy π^* in $O(n^2m/(1-\gamma))$ iterations (converges in polynomial number of iterations)!

6.3 Value iteration (Cost $O(SA\Delta)$)

Initialize $V_0(x) = max_a r(x,a)$
For $t = 1$ to ∞:
- For each (x,a), let:
$Q_t(x,a) = r(x,a) + \gamma\sum_{x'} P(x'|x,a)V_{t-1}(x')$
- For each x, let $V_t(x) = \underset{a}{max} Q_t(x,a)$
- Break if $\|V_t - V_{t-1}\|_\infty = \underset{x}{max}|V_t(x) - V_{t-1}(x)| \le \epsilon$

Then choose greedy policy w.r.t V_t.
Guaranteed to converge to ϵ-optimal policy (finds approximate solution in polynomial number of iterations)!

6.4 POMDP = Belief-state MDP

States = beliefs over states for original POMDP
$B = \Delta(1,...,n) = \{b : 1,...,n \to [0,1], \sum_x b(x) = 1\}$
Actions: same as original MDP
Transition model:
- Stochastic observation:
$P(Y_t|b_t) = \sum_{x=1}^n P(Y_t|X_t = x)b_t(x)$
- State update (Bayesian filtering!), given b_t, y_t, a_t: $b_{t+1}(x') = \frac{1}{Z}\sum_x b_t(x)P(y_t|x)P(X_{t+1} = x'|X_t = x, a_t)$

Reward function: $r(b_t, a_t) = \sum_x b_t(x)r(x,a_t)$

6.5 Example of approx. solution to POMDPs: Policy gradients

- Assume parameterized policy: $\pi(b) = \pi(b;\theta)$
- For each parameter θ the policy induces a Markov chain
- Can compute expected reward $J(\theta)$ by sampling.
- Find optimal parameters through search (gradient ascent): $\theta^* = \underset{\theta}{argmax}\ J(\theta)$

7 Learning models from training data

7.1 Learning from i.i.d data

Algorithm for Bayes Net MLE:
Given BN of structure G and dataset D of complete observations
For each X_i estimate: $\hat\theta_{X_i|Pa_i} = \frac{Count(X_i, Pa_i)}{Count(Pa_i)}$
Pseudo-counts for lime and cherry flavor: $\theta_{F=c} \frac{Count(F=c)+\alpha_c}{N+\alpha_c+\alpha_l}$

7.1.1 Score based structure learning

Define scoring function $S(G;D)$ and search over BN structure G: $G^* = \underset{G}{argmax} S(G;D)$

Examples of scores:
MLE Score:
$logP(D|\theta_G, G) = N\sum_{i=1}^n \hat I(X_i; Pa_i) + const.$
Where mutual information $(I(X_i, X_j) \ge 0)$ is:
$I(X_i, X_j) = \sum_{x_i,x_j} P(x_i,x_j)log\frac{P(x_i,x_j)}{P(x_i)P(x_j)}$
Empirical mutual information:
$\hat P(x_i,x_j) = \frac{Count(x_i,x_j)}{N}$
$\hat I(X_i,X_j) = \sum_{x_i,x_j} \hat P(x_i,x_j)log\frac{\hat P(x_i,x_j)}{\hat P(x_i)\hat P(x_j)}$
Regularizing a Bayes Net:
$S_{BIC}(G) = \sum_{i=1}^n \hat I(X_i; Pa_i) - \frac{logN}{2N}|G|$
where G is the number of parameters, n the number of variables and N the number of training examples.
Chow-Liu algorithm:
- For each pair X_i, X_j of variables, compute: $\hat P(x_i,x_j) = \frac{Count(x_i,x_j)}{N}$
- Compute mutual information
- Define complete graph with weight of edge (X_i, X_j) given by the mutual information
- Find max spanning tree $\to$ undirected tree
- Pick any variable as root and orient the edges away using breadth-first search.

8 Reinforcement Learning

8.1 Model-based RL

8.1.1 ϵ greedy

With probability ϵ, pick random action. With prob $(1-\epsilon)$, pick best action. If sequence ϵ satisfies Robbins Monro criteria $\to$ convergence to optimal policy with prob 1.

8.1.2 R_{max} algorithm

Input: starting x_0, discount factor γ.
Initially: add fairy tale state x^* to MDP
- Set $r(x,a) = R_{max}$ for all states x and actions a
- Set $P(x^*|x,a) = 1$ for all states x and actions a
- Choose the optimal policy for r and P

Repeat: 1. Execute policy π and, for each visited state/action pair, update $r(x,a)$
2. Estimate transition probabilities $P(x'|x,a)$
3. If observed 'enough' transitions/rewards, recompute policy π, according to current model P and r.
Enough"? See Hoeffding's inequality. To reduce error ϵ, need more samples N.
Theorem: With probability $1-\delta$, R_{max} will reach an ϵ-optimal policy in a number of steps that is polynomial in $|X|, |A|, T, 1/\epsilon$ and $log(1/\delta)$.
Memory $O(|X^2||A|)$.

8.2 Model-free RL: estimate V*(x) directly

8.2.1 Q-learning

$Q(x,a) \leftarrow (1-\alpha_t)Q(x,a) + \alpha_t(r + \gamma\max_{a'} Q(x',a'))$
Theorem: If learning rate α_t satisfies: $\sum_t \alpha_t = \infty$ and $\sum_t \alpha_t^2 < \infty$ (Robbins-Monro), and actions are chosen at random, then Q learning converges to optimal Q^* with probability 1.
Optimistic Q learning:
Initialize: $Q(x,a) = \frac{R_{max}}{1-\gamma}\prod_{t=1}^{T_{init}}(1-\alpha_t)^{-1}$
Same convergence time as with R_{max}. Memory $O(|X||A|)$. Comp: $O(|A|)$.
Parametric Q-function approximation: $Q(x,a;\theta) =^T \phi(x,a)$ to scale to large state spaces. (You can use Deep NN here!)
SGD for ANNs: initialize weights. For t = 1,2..., pick a data point (x,y) uniformly at random. Take step in negative gradient direction. (In practise, mini-batches).
Deep Q Networks: use CNN to approx Q function. $L(\theta) = \sum_{(x,a,r,x')\in D}(r + \gamma\underset{a'}{max}Q(x',a';^{old}) - Q(x,a;))^2$ **Double DQN:** current network for evaluating argmax (too optimistic, and you remove θ^{old} and put θ).

8.3 Gaussian processes

A GP is an (infinite) set of random variables (RV), indexed by some set X, i.e., for each x in X, there is a RV Y_x where there exists functions $\mu : X \to \mathbb{R}$ and $K : X \times X \to \mathbb{R}$ such that for all: $A \in X$, $A = x_1, ...x_k$, it holds that $Y_A = [Y_{x_1}, ..., Y_{x_k}] \sim N(\mu_a, \Sigma_{AA})$, where: Σ_{AA} = matrix with all combinations of $K(x_i, x_j)$.
K is called kernel (covariance) function (must be symmetric and pd) and μ is called mean function. **Making prediction with GPs:** Suppose $P(f) = GP(f;\mu,K)$ and we observe $y_i = f(\vec{x_i}) + \epsilon_i$, $A = \{\vec{x_1} : \vec{x_k}\}$ $P(f(x)|\vec{x_1} : \vec{x_k}, y_{1:k}) = GP(f;\mu',K')$. In particular, $P(f(x)|\vec{x_1} : \vec{x_k}, y_{1:k}) = N()f(x);\mu_{x|A}, \sigma^2_{x|a}$, where $\mu_{x|a} = \mu(\vec{x}) + \Sigma_{x,A}(\Sigma_{AA} + \sigma^2 I)^{-1}\Sigma_{x,A}^T(\vec{y_A} - \mu_A)$ and $\sigma^2_{x|a} = K(\vec{x},\vec{x}) - \Sigma_{x,A}(\Sigma_{AA} + \sigma^2 I)^{-1}\Sigma_{x,A}^T$.
Closed form formulas for prediction!